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Ron Fedkiw

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Stanford University
651 Serra St.
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Reza Malek-Madani
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Algorithm Design for Computational Fluid Dynamics, Scientific Visualization and Image Processing
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#14 ABSTRACT

We developed a novel approach to extend the particle level set method to the simulation of as many regions as desired. The various regions can be liquids or gases of any type with differing viscosities, densities, viscoelastic properties, etc. We also proposed techniques for simulating interactions between materials, whether it be simple surface tension forces or more complex chemical reactions with one material converting to another or two materials combining to form a third. When discretizing the underlying Navier-Stokes equations for multiphase flow, an additional difficulty occurs since discretization stencils cross region boundaries naively combining non-smooth or even discontinuous data. Recently, we developed a new coding paradigm that allows one to incorporate physical jump conditions in data ``on the fly," which is significantly more efficient for multiple regions especially at triple points or near boundaries with solids. This removes the need for any algorithm changes that might reduce the accuracy of the scheme, and moreover even removes the need for changes to the code itself. Besides this work we have also addressed scalability including methods on octree and Run Length Encoded (RLE) data structure, as well parallel implementation such as MPI. Other work includes work on fracture.

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Algorithm Design for Computational Fluid Dynamics, Scientific Visualization and Image Processing

N00014-01-1-0620-P00006

Ronald Fedkiw
Stanford University, Computer Science Department

The particle level set method [EFFM,EMF] was developed under prior ONR funding, and has proven successful for the numerical simulation of two separate regions. In the case of free surfaces, the Dirichlet boundary conditions imposed on the water/air boundary were increased to second order accuracy in [ENGF] using the technique proposed in [GFCK]. Later, [ELF] showed that the level set advection could be handled with a simple first order accurate semi-Lagrangian method as long as the particles were advected with second order accuracy. This allowed for the extension of the method to more complex phenomena, such as coupling to thin deformable objects as in [GSLF]. This plays a key role in a recent MURI in which Farhat and Fedkiw compose the Stanford team. This work on coupling two phase flows to both rigid and deformable solids leveraged our recent algorithms for rigid body simulation [GBF], and finite element simulation of deformable volumetric bodies [ITF] and thin shells [BFA]. We even developed numerical techniques that allowed a deformable solid modeled with a Lagrangian finite element mesh to phase change into a liquid modeled with an Eulerian background mesh. However, all of these algorithms were still limited to at most two liquid phases.

Thus, most recently we developed a novel approach to extend the particle level set method to the simulation of as many regions as desired [LSSF]. The various regions can be liquids or gases of any type with differing viscosities, densities, viscoelastic properties, etc. We also proposed techniques for simulating interactions between materials, whether it be simple surface tension forces or more complex chemical reactions with one material converting to another or two materials combining to form a third. We use a separate particle level set method for each region, and propose a novel projection algorithm that decodes the resulting vector of level set values providing a ``dictionary'' that translates between them and the standard single-valued level set representation.

When discretizing the underlying Navier-Stokes equations for multiphase flow, an additional difficulty occurs since discretization stencils cross region boundaries naively combining non-smooth or even discontinuous data. Under previous ONR funding, we introduced the ghost fluid method [FAMO] some years ago in order to treat this problem for compressible flow. Sine then, it has been extended to incompressible flows [LFK,KFL] and combustion [NFK,NFJ] and addressed by many other authors. Although the original idea in [FAMO] was to create ghost cells, many authors have explored various algorithm or implementation ideas to avoid the ghost cells with the aim of achieving identical or at least similar results. In [LSSF], we developed a new coding paradigm that allows one to incorporate physical jump conditions in data ``on the fly,'' which is significantly more efficient for multiple regions especially at triple points or near boundaries with solids. This removes the need for any algorithm changes that might reduce the accuracy of the scheme, and moreover even removes the need for changes to

the code itself. A smart discretization class is used to encode both the region one is working in as well as the required jump conditions, and the programmer simply writes the code as if it were for a single region relying on the smart discretization class to create the correct code.

Computational resources are almost always limited, and this problem cannot typically be addressed by getting more machines as the algorithms do not always scale to multiple processors. Thus, there is a variety or research into way of improving the efficiency of the algorithms themselves such as adaptive mesh technology. In fact, under ONR funding, we proposed first algorithms for multiphase flow simulation on an octree data structure in [LGF]. Later in [LGO], we both extended our discretization to second order accuracy as well as proposing a more efficient technique that uses a top level Cartesian grid placing an individual octree in each Cartesian cell. Most recently we have examined methods for discretizing large bodies of water where researchers typically use either the deep water or shallow water approximations. We instead wanted to use a fully three dimensional technique to capture wave overturning and related effects, but obviously had to use an adaptive mesh because of computational limitations. Instead of using the octree or a patch based AMR approach, we designed a new method based on Run Length Encoding (RLE) from image processing. RLE takes an image of pixels, and compresses them by storing row subsets with similar properties in a smaller data structure. Applying the same idea to the incompressible Navier-Stokes equations, we start with a uniform Cartesian grid and merge any two or more cells in order to make tall cells. Note that we only merge cells in the vertical direction, since we will be treating pressure linearly in each of these cells, and a linear pressure profile is more valid in water than a linear horizontal one. In fact, if every column of water were merged into one cell, we would obtain a two-dimensional height field approximation similar to the shallow water equations. Thus we typically merge parts of columns under water while leave fully three-dimensional approximations near the surface of the water and near any objects (which may be submersed). Starting with the standard MAC grid discretization of the incompressible Navier-Stokes equations, [IGLF] develops the natural discretizations obtained by merging cells in this vertical fashion assuming linear pressure profiles. A current limitation of the merged tall cells is that they cannot adequately resolve vorticity. However, we have also recently developed a hybrid simulation framework that leverages a vortex particle approach on a background grid [SRF]. This method can also be exteneded to properly carry vorticity through the merged tall cells.

In addition to adaptive mesh strategies, we have been working on ways to make algorithms more scalable. Recently, our group was awarded a DURIP which was used to purchase an 80 processor SUN with 600G of RAM. Since obtaining the cluster, we have worked to parallelize our code base using MPI and currently have the full fluid simulation system parallelized. Also, both the PI and two graduate students involved in this work received screen credits on the film Poseidon – which has been nominated for an Oscar for special effects work. For that film, Industrial Light + Magic made used of our new MPI code base to simulate all of the ocean scenes. In that film, the entire ship and ocean were completely computer generated using our PhysBAM software. Of course, it is not enough to merely write the MPI code, but rather one needs to find the bottlenecks and

improve the implementation – or even create better algorithms. Thus, we have been collaborating with Intel for some time working on getting algorithms from our PhysBAM code based implemented in their multicore framework. Two students from our group spend one day at Intel on a weekly basis. Intel is pushing for a suite of new multicore benchmarks and our code base will be part of this. Currently, we our working on extending our finite element solids simulations to the MPI frame work as well.

Previously, we have done quite a bit of work on the finite element simulation of solids, some of which is mentioned above. The early work focused on using level set methods to create red-green adaptive tetrahedral and surface triangle meshes for subsequent finite element simulation [MBTF,BTMF]. Our main interest was in contact and collision, as well as materials that undergo large deformation, plasticity and fracture. Thus, a main concern was that the finite element technique would be robust under large deformation and we devised a new algorithm in [ITF] that not only allowed tetrahedral to invert, but that provided forces that would work to un-invert them. When materials fracture, it becomes necessary to generate a new mesh for the finite element analysis. Thus, we proposed a new virtual node algorithm to automatically generate this mesh in [MBF]. This method has a similar flavor to the ghost fluid method where ghost nodes are created to model discontinuities in the material. The main contribution of the algorithm is that it figures out exactly how to most efficiently treat all the degrees of freedom by creating ghost nodes as parts of new tetrahedral. As far as this aspect of the algorithm is concerned, it turns out that XFEM is a subset of our approach. Once these new degrees of freedom are created, one can proceed in almost standard fashion with a robust and efficient finite element mesh. Most recently, in [BHTF], we have extended our prior work on fracture to treat truly rigid bodies that can fracture into multiple rigid bodies. Some of the key aspects of the approach included a method to properly handle the null space in the rigid body finite element simulation as well as techniques for treating the subsequent contact and collision.

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